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High-pressure compressibility and thermal expansion of aragonite

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ABSTRACT

The structure and isothermal equation of state of aragonite were determined to 40 GPa using synchrotron single-crystal X-ray techniques. In addition, powder diffraction techniques were used to determine thermal expansion between 298–673 K. At room temperature, aragonite has orthorhombic Pnma structure to 40 GPa, with an isothermal bulk modulus of 66.5(7) GPa and $K' = 5.0(1)$. Between 25–30 GPa the aragonite unit cell begins to distort due to a stiffening of the *c*-axis compressibility, which is controlled by the orientation and distortion of the carbonate groups. The ambient pressure thermal expansion measurements yielded thermal expansion coefficients $a_0 = 4.9(2) \times 10^{-5}$ and $a_1 = 3.7(5) \times 10^{-8}$. The combined results allow the derivation of a thermal equation of state. The new data provide constraints on the behavior of carbonates and carbon cycling in the Earth's crust and mantle.

Keywords: Aragonite, high pressure, thermal expansion, compressibility, equation of state, single crystal, X-ray diffraction